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May 13, 2022

RESEARCH AND EXPLORATORY DEVELOPMENT  
REDD-2022-327

DARPA/I2O  
675 North Randolph Street  
Arlington, VA 22203-2114

Attention: Dr. Joshua Elliott

Subject: DARPA PACMANS Milestone 4 (Tasks 3.3 and 4.3): Report on 'beta version' of hybrid model analysis including new mathematical insights, along with insights in data analysis

Reference: (a) Contract HR00112290032 Task Order HR0011256743, The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

Attachment(s): (1) DARPA PACMANS Milestone 4 Report (Contractor Task Number VQE70)

Dear Dr. Elliott:

The Johns Hopkins University Applied Physics Laboratory (JHU/APL) is pleased to provide the Milestone 4 Report for PACMANS under Contract HR00112290032 Task Order Number HR0011256743. The enclosure includes JHU/APL proprietary information that shall not be discussed outside DARPA.

If you have any questions or comments, please contact me at (240) 228-9433 or via e-mail [@Marisa.Hughes@jhuapl.edu](mailto:@Marisa.Hughes@jhuapl.edu).

Sincerely,

Marisa J. Hughes, PhD.  
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# The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery Milestone 4 Report

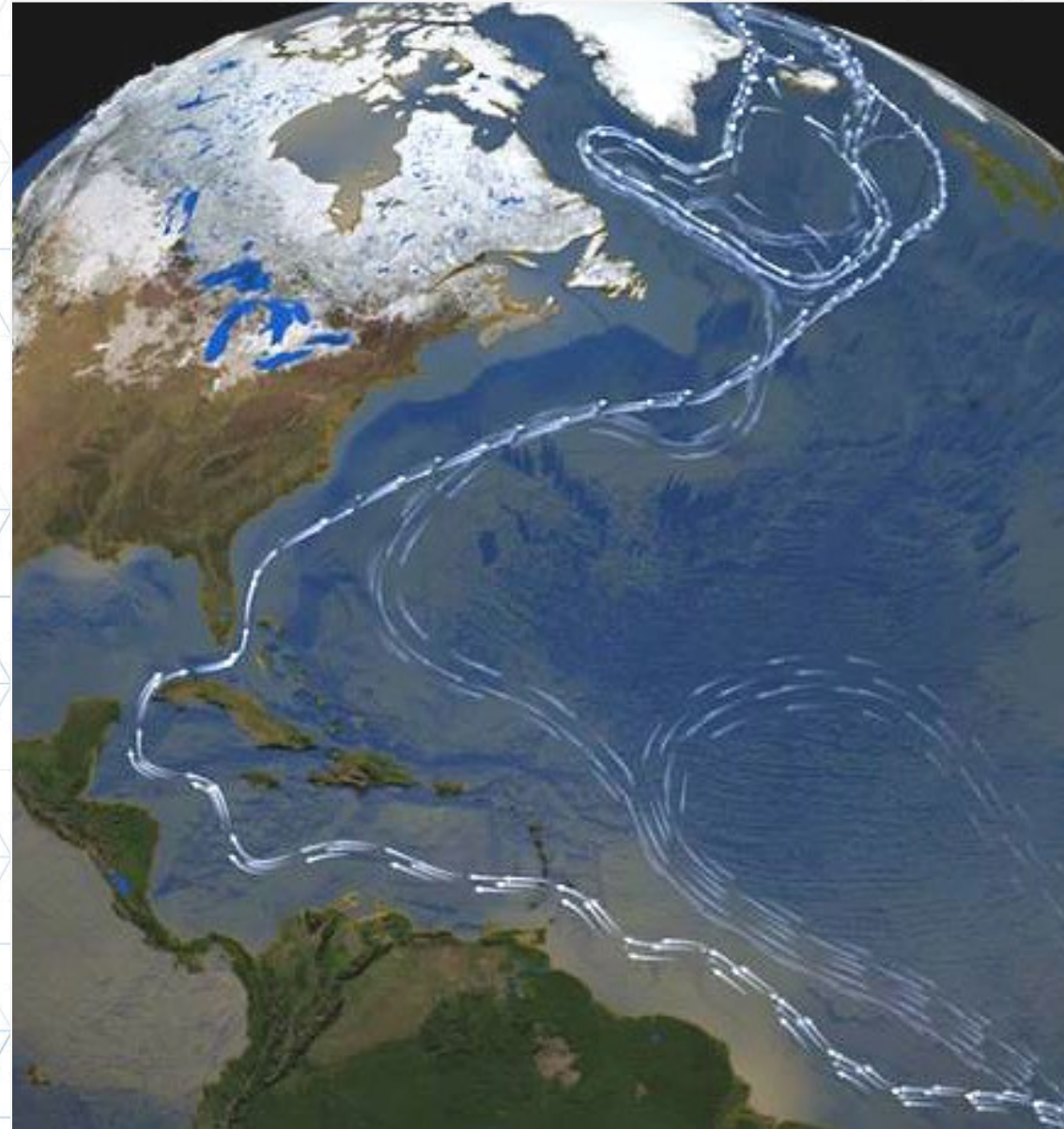
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# Overview

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- This technical report covers the period of April 2022 through May 13, 2022.
- The report documents the achievement of the milestone associated with Month 5 of the JHU/APL-led PACMAN team's statement of work.
- The delivery for this milestone is this report which highlights progress made for the AI surrogate modeling and the AI simulation research.
- This report includes:
  - New architectures
  - Experimental definitions
  - Findings based on experimental results
  - Next steps

# Goals and Impact

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

Goals for this milestone included:

- Obtain the first set of experimental results for the AI surrogate modeling based on testing the formalizations described in Milestone 3
- Perform early experimentation of a baseline GAN for a subset of explorations and what-if questions
  - Show feasibility of the causal model
  - Obtain baseline symbolic language experimental results

# Key Findings

## The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- Surrogate Learning (Task 3.3)
  - Completed the first set of bifurcation diagrams for the box model equations
  - Discovered a new type of tipping point in the Box model using the non-dimensionalized equations
    - In Gnanadesikan 2018 paper a fold bifurcation was assumed, we discovered subcritical Hopf bifurcation also exists for the reverse transition
    - **Plan to publish these findings – this represents a new insight into potential AMOC behavior**
- AI simulation (Task 4.3)
  - Completed first set of multi-agent generator GAN experiments using the box model data
    - **Generators show a positive tendency towards AMOC collapse**
  - Setup a baseline neuro-symbolic experiment using rules-based model with a set of questions which correlate with the box model Gnanadesikan 2018 experiments
  - Developed a first approach for bi-directional translation between the neuro-symbolic language and the GAN perturbations
    - **If successful, this model will show how a GAN's perturbations of symbols can be translated to “purely generative” natural language questions**
  - To address questions around AMOC slowing vs. complete shut-off and recovery from AMOC, we are exploring causality at the model level
    - **we expect to address these two areas with a probabilistic causal model**



## Task 3.3 – Surrogate Learning Summary

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

*Subtask Description: Report on the first set of experimental results based on testing the formalizations set forth in Milestone 3.*

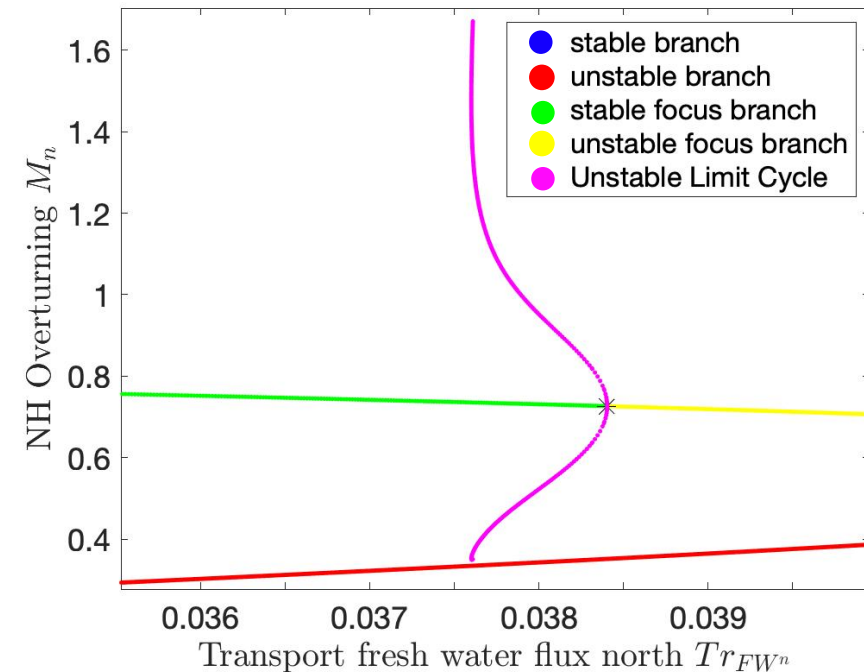
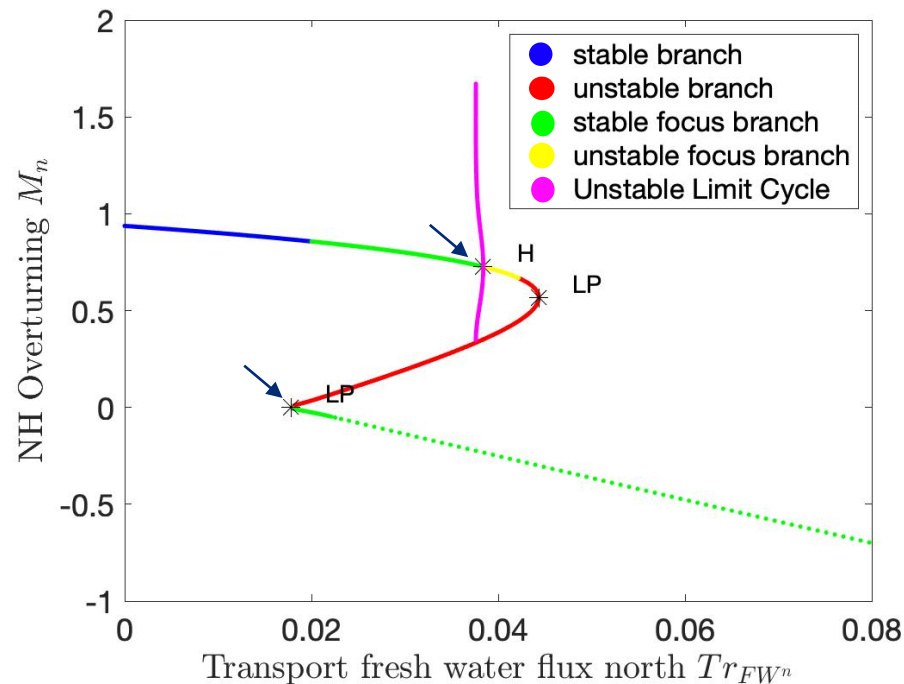
Accomplishments:

- **Major breakthrough** in terms of bifurcation modeling
  - We have been able to perform detailed bifurcation diagrams of the box model
  - This was enabled by a careful non-dimensionalization of the related equations, without which the accuracy of the numerical computations would be unsatisfactory
  - With the non-dimensionalized equations, the problem possesses not one but two tipping points (fold and Hopf bifurcations)

## Task 3.3 - Surrogate Learning

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

With the non-dimensionalized equations, the problem possesses not one but two tipping points (from the “upper” branch to the lower, but also from the lower to the upper) as shown in Figures 1-2.



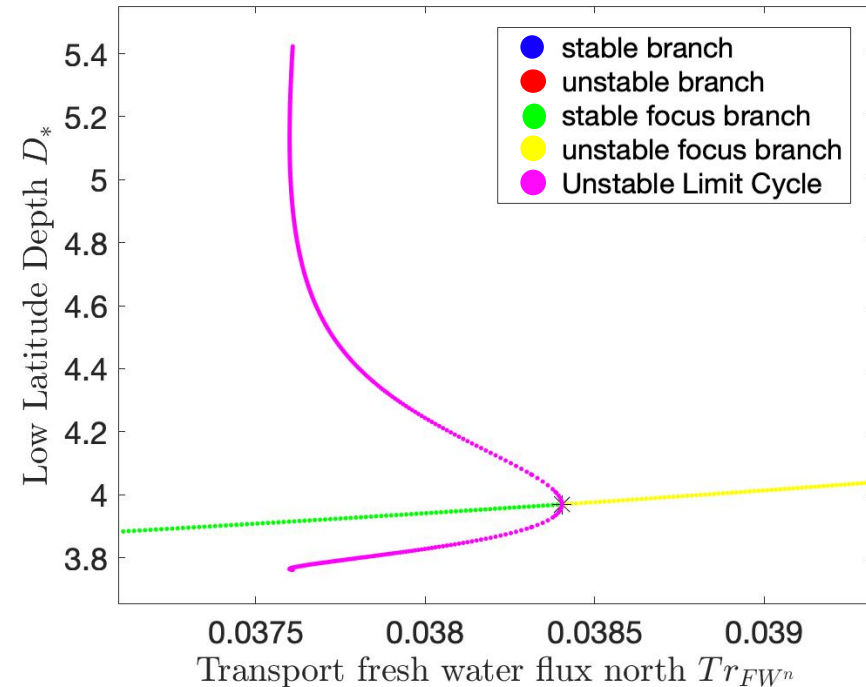
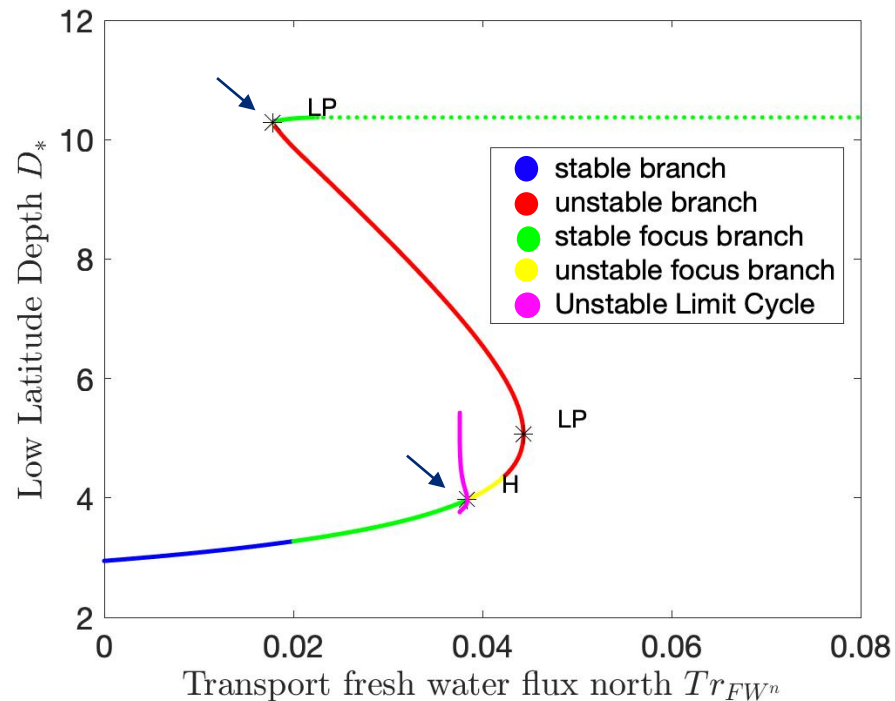
Figures 1a-1b. Diagram of NH Overturning  $M_n$  (a) and Zoomed-In View of the subcritical Hopf Bifurcation Point (b).



## Task 3.3 - Surrogate Learning

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

Second view - the two tipping points are of different nature: one of the two is the fold point bifurcation, but the second one is a subcritical Hopf, highlighted in Figures 1-2. The Hopf at  $Tr_{FW}^n=0.0384$  is subcritical.



Figures 2a-2b. Diagram of Low Latitude Depth  $D_*$  (a) and Zoomed-In View of the Hopf Bifurcation Point (b).

## Task 3.3 - Surrogate Learning

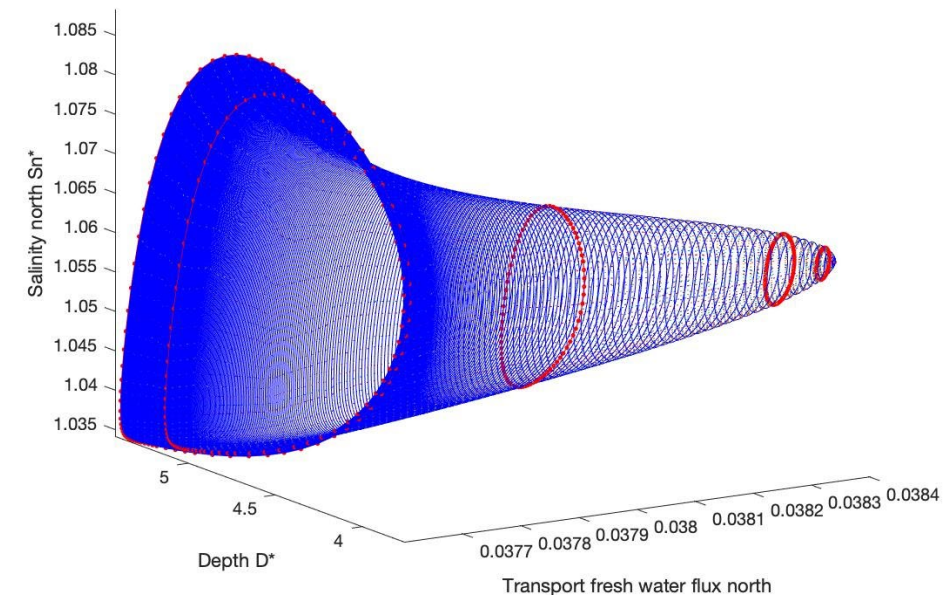
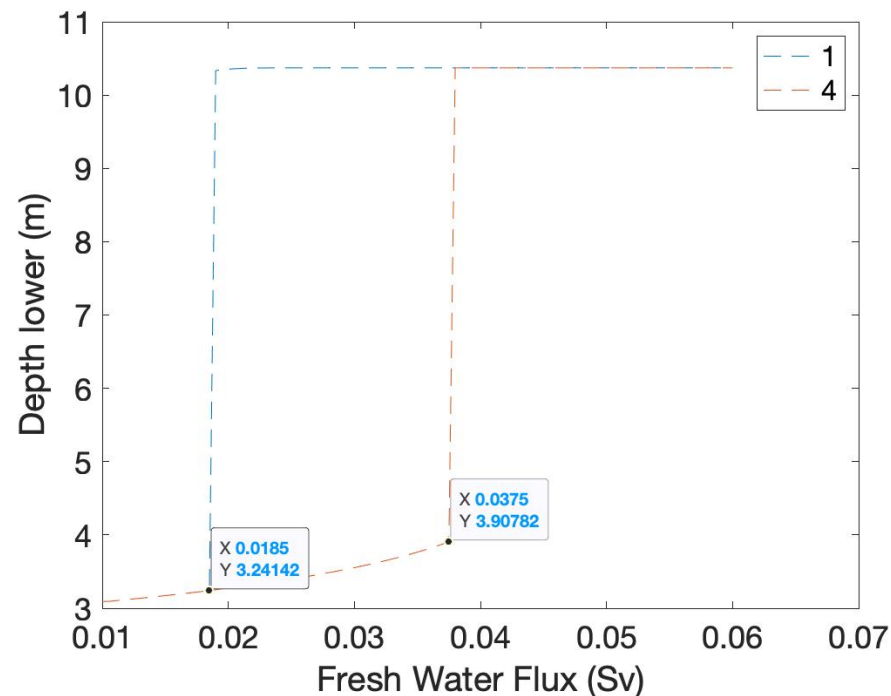
The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- The value where the limit cycle branch appears to become vertical (an infinite period, homoclinic orbit) is 0.0375.
- The subcritical Hopf gives birth to an unstable limit cycle “backwards” in parameter space (that surrounds the exiting stable steady state).
- This steady state loses stability at the Hopf bifurcation (red branch in Figures 1-2).
- The escape (the “tipping”) arises when a stochastic trajectory wandering around the stable state manages to “cross” the unstable limit cycle and escape to either large oscillations or to a completely different lower circulation branch.

## Task 3.3 - Surrogate Learning

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

Where the initial condition with  $D=1$  (where  $D$  is the Low latitude pycnocline depth) is attracted by the upper branch because there is an early switch activation, so the sharp transition that we see is given by the upper limit point LP. While for  $D=4$  we observe the sharp transition close to the subcritical Hopf (the solution loses stability at the exact Hopf point, because the initial condition may start outside the unstable limit cycle).



Figures 3a-3b. Temporal Bifurcation Diagram for Depth (a) and the Limit Cycle Continuation (b).

## Task 3.3 - Surrogate Learning

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

### Next Steps:

- We are working on a stochastic simulation close to the presented tipping points, to collect data towards a targeted surrogate model. This will allow us to efficiently and accurately estimate escape time distributions.
- We will learn targeted effective stochastic DEs (one-dimensional at the LP tipping, two-dimensional at the Hopf tipping) and use them to estimate escape time statistics in both cases.

## Task 4.3 – AI Simulation Summary

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

*Subtask Description: Report on early experimentation of a baseline GAN for a subset of explorations and what-if questions, including a set of experiments that show feasibility of the causal model, and baseline symbolic language experimental results.*

Accomplishments:

- Started conducting GAN experiments using the box model data
  - Exploring behavior of multi-agent GAN loss function
  - Exploring optimal number of generators
- Developed architectures needed for a baseline neuro-symbolic language that enables a translation from human-specific questions to the GAN simulation, and from perturbed GAN runs to questions.
  - Set up a baseline model that will be used for experimentation
- Defined causality in terms of model behavior/time

## Task 4.3 - AI Simulation – GAN Experiments

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- Three experiments using the Box model simulation data
- With a vector of 3 dimensions and perturbations of parameters (bounded):
  - Dlow0 (Thermocline depth of lower latitudes): [100.0, 400.0]
  - Mek (Ekman flux from the southern ocean): [1.5e7, 3.5e7]
  - Fwn (Fresh water flux (North)): [5.0e4, 1.55e6]
- Data was augmented for uniform sampling from a 3-D space
- In addition to samples, generated 1,000 synthetic samples
  - Distribution of shutoff vs non-shutoff samples 743/413



## Task 4.3 - AI Simulation – GAN Experiments

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- Trained the GAN using equally-weighted generators
- Shutoff classification cross-entropy loss functions
- Ran for ~250 epochs
- Ran experiments with  $n$  = to the number of generators where  $n \in [1, 2, 4]$
- Generated samples result in shutoffs/non-shutoffs

## Task 4.3 - AI Simulation – GAN Experiments

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- Discriminator performance in classifying runs as shut-off or not
- High F-measure scores indicate the discriminator was able to accurately classify shut-off from non-shut-off runs for held-out test set

Table 1. Precision, Recall, F-Measure scores for 1,2,4 generator GANs.

	<i>Precision</i>	<i>Recall</i>	<i>F-Measure</i>
<b>1 Generator</b>	1	1	1
<b>2 Generators</b>	0.993	1	0.997
<b>4 Generators</b>	0.929	1	0.963

Small initial experiment- but very promising results from discriminator in classifying runs

## Task 4.3 - AI Simulation – GAN Experiments

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- After training the GAN, sampled 500 times
- Generators tend to favor exploring areas of shut-offs
  - Training data had some imbalance
  - Larger dataset would provide verification

Table 2. For 1,2,4 generator GANs – Fraction of 500 samples that resulted in a shut-off.

		Generator Idx			
		0	1	2	3
Number of Generators	1	0.854	n/a	n/a	n/a
	2	0.992	0.998	n/a	n/a
	4	0.982	0.986	0.972	1

The trained generators are successfully generating a latent space of shut-offs

# Task 4.3 - AI Simulation – GAN Experiments

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- Early GAN results show interesting results regarding  $M_n$  and shut-off behavior. More experimentation is underway to explore this further.

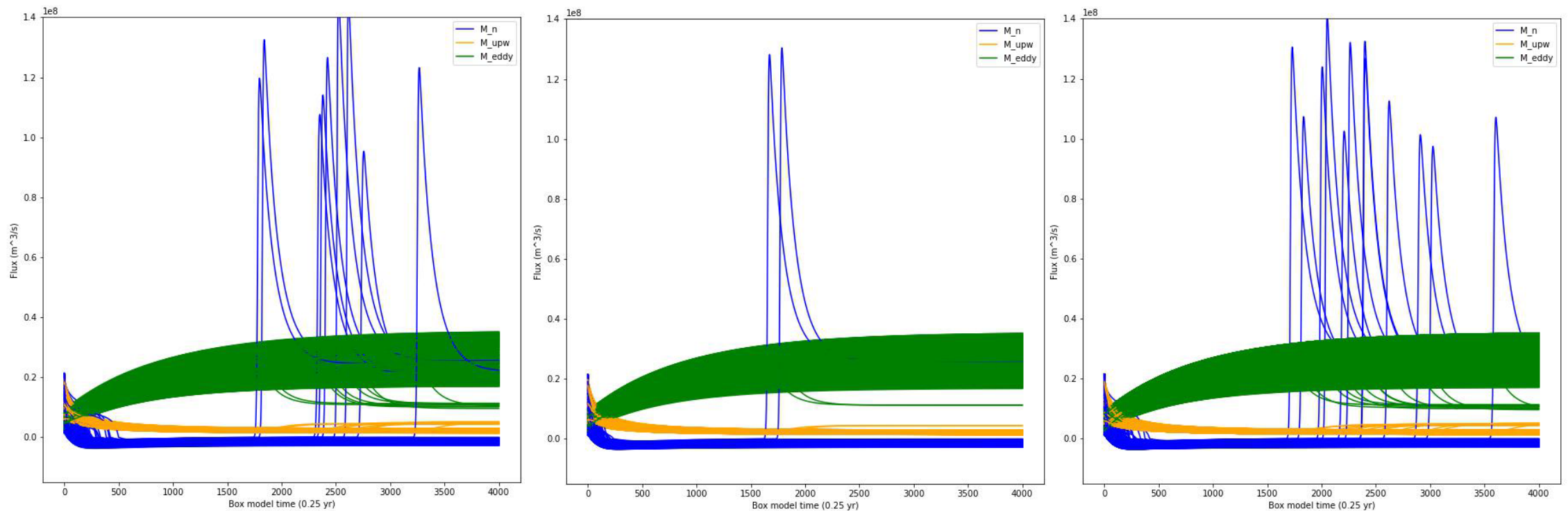


Figure 4a-c. GAN generated shut-offs for 1 generator (a), 2 generators (b), and 4 generators (c).

## Task 4.3 - AI Simulation – GAN Experiments

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

### Observations:

- The  $n=1$  generator case produces the greatest fraction of configurations that are non-shutoff states. This could be attributed to the GAN having more synthetic samples to learn from (i.e.  $n=2$  and  $n=4$  training loops versus  $n=1$  training loop per epoch).
- For this particular scenario (i.e. 3 perturbed features w/ fixed bounds), it appears that  $n=1$  generator is enough to roughly capture the shutoff configurations in this feature space. However, it's still to be determined how the generators will perform when allowed to perturb more than 3 features.

## Task 4.3 - AI Simulation – GAN Experiments

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- For Fwn the  $n=1$  generator GAN learns a bi-modal sampling distribution with modes centered at approx..  $0.65e6$  and  $1.3e6$ .
- When  $n=2$  or  $n=4$ , generators learns a left-skewed uni-modal sampling distribution with mode centered at approx..  $1.3e6$ .

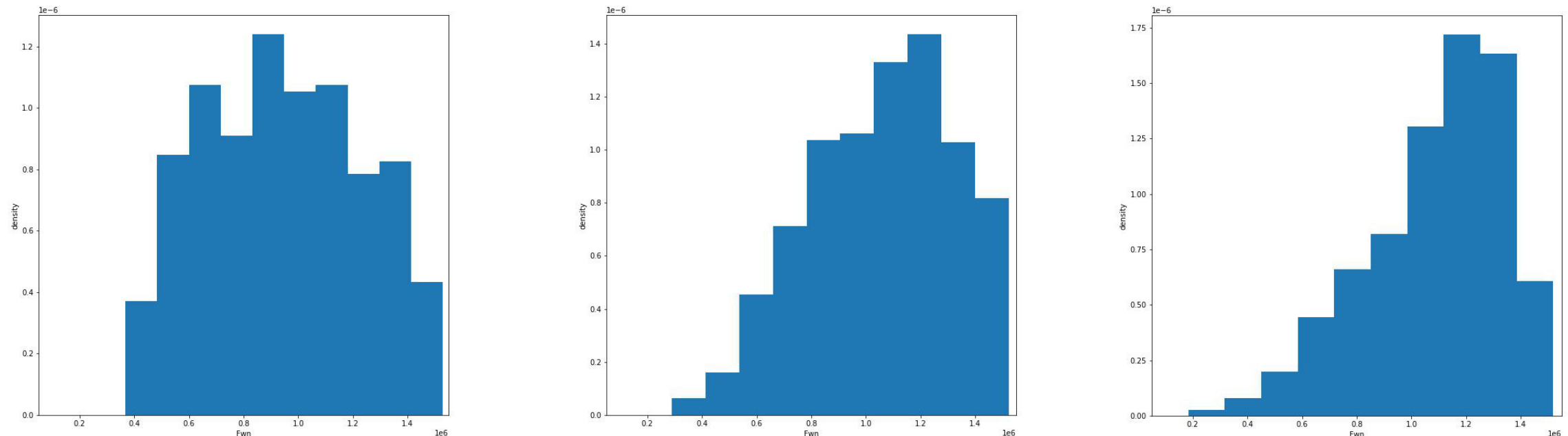


Figure 5a-c. Histograms showing distribution of generated shut-offs for 1 generator (a), 2 generators (b), and 4 generators (c).



## Task 4.3 - AI Simulation – GAN Experiments

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

### Observations:

- The mode at  $0.65e6$  has a large cluster of non-shutoff states, while the mode at  $1.3e6$  appears to be a cluster for a shutoff state. This finding also coincides with the larger fraction of non-shutoff states generated by the  $n=1$  GAN vs.  $n=2$  and  $n=4$  GANs.
- Discriminators incorrectly classify a larger fraction of real samples as synthetic as the number of generators increases.

# Task 4.3 - AI Simulation – Neuro-Symbolic Learning

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

Neuro-symbolic architecture has been defined in terms of levels of representation:

- Text level – climate modeler asks questions
- Symbolic level – “programs” generated from natural language
- Vector level – GAN works at vector-level perturbing parameters
- Model level – Surrogate receives input in terms of initial conditions and parameters to run model

## Levels of Representation Overview

Does the stability of the overturning depend on the pathways and sensitivities of water mass transformation in the Southern Ocean?

Text Level

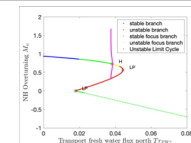
Query(Overturning\_Stability, Relate(Filter(Water Mass Transformation), filter(Southern Ocean)))

Symbolic Level

$v_1$   $v_2$   $v_3$

Vector Level

When the GAN randomly generates a configuration – this should be translatable into a question or set of questions



GAN will call on surrogate to determine if perturbation is a shut-off

Model Level

**Figure 6. Levels of Representation from Natural Language to Model runs.**

# Task 4.3 - AI Simulation – Neuro-Symbolic Learning

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- In training mode: GAN explores space through perturbations
- Perturbations are translated into “programs”
- “Programs” are translated into natural language
- In trained mode: Questions can be asked of the model
- Questions are translated into ‘programs’
- ‘Programs’ are used to find answers using latent space

## Training Mode:

Let GAN explore space?  
Have a way to convert from parameter vectors to symbolic translation to questions  
They will be found in a latent space built by the GAN  
However an embedded space will tell us something about similarity of questions

## Trained Mode:

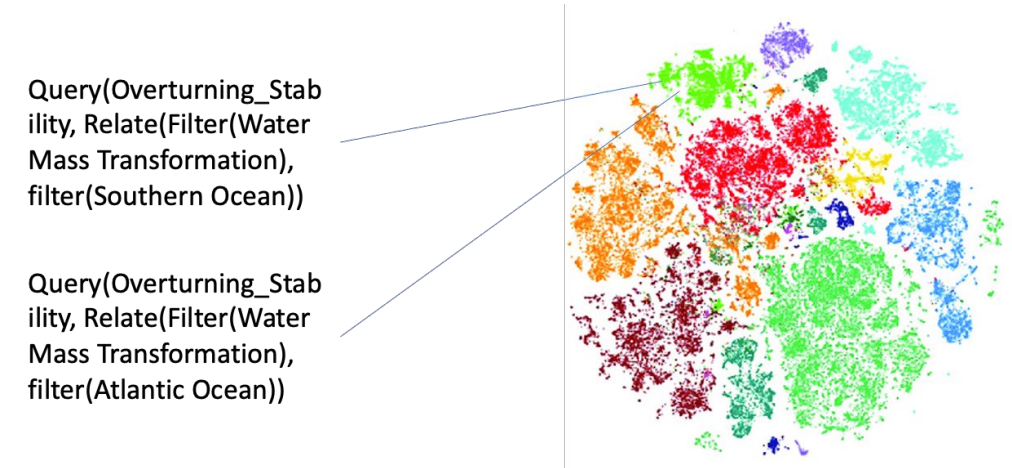
Ask questions  
Convert questions to symbolic translations, use the embedding space to obtain confidence in the translation  
Convert translations into vectors, use vectors to find answers to questions to latent space.

**Figure 7. Training vs. Trained Mode and AI vs. Human Question and Answers.**

# Task 4.3 - AI Simulation – Neuro-Symbolic Learning

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- Programs are embedded in a latent shared space with the GAN
- GAN perturbations and human-generated questions can be bi-directionally translated using this space
- Question “programs” similar to each other will be embedded near each other in this space



**Figure 8.** Notional low dimensional embedding of “programs” that represent natural language questions.

# Task 4.3 - AI Simulation – Neuro-Symbolic Learning

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- **Designed a question template for experimentation**
- Simple template as shown in Figure 9a
- Will be used as a first version of questions for training networks
- Questions are generated similar to the example question in Figure 9b
- These questions correlate tightly to the box model experiments and also with the GAN experiments

(a) **Question form**

"If one sets <BMI> to <VALUE> (and <BMI> to <VALUE>...), will <FUNCTION> on <BMO>?"

- **BMI:** Box Model Input (e.g. "Fwn", "T\_south0", "D\_low", etc.)
- **VALUE:** Numeric value
- **FUNCTION:** Man made functions that operate on BMOs
- **BMO:** Box Model Output (e.g. "M\_n")

(b) **Example Question**

"If one sets Fwn to 10000 and N to 1000, will ChangeSign on M\_n?"

- Fwn: Freshwater flux in the norther hemisphere
- N: Number of time steps to run the box model
- ChangeSign: Does a given 1D array contain both positive and negative values?
- M\_n: Northern Hemisphere overturning

Figure 9a-b. Question Template for Version 1 of Neuro-symbolic language (a) and Example Question Using this Template (b).

## Task 4.3 - AI Simulation – Neuro-Symbolic Learning

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

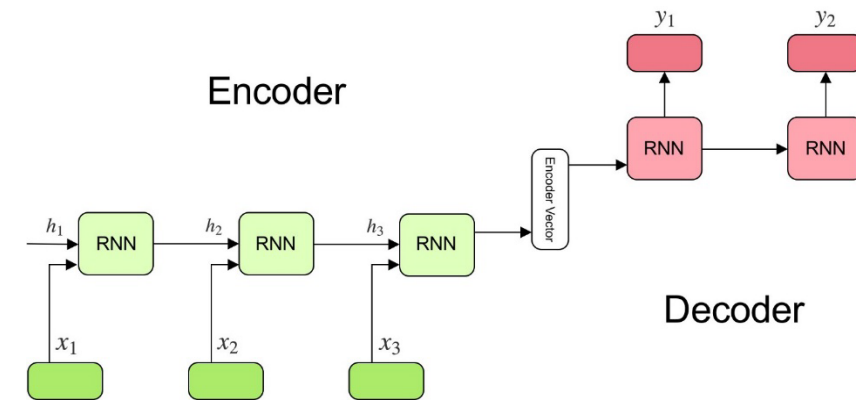
- **Have currently developed a rule-based method that generates encodings of questions as “programs”**
- Based on a defined Domain Specific Language (DSL)
- Will be used as a baseline for evaluating deep learning methods
- Built an automatic question generator for questions following the form in Figure 9a.



# Task 4.3 - AI Simulation – Neuro-Symbolic Learning

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- Experimenting with a sequence-to-sequence autoencoder to encode questions, and decode into vector input for a GAN
- Based on a sequence-to-sequence machine translation
- Includes an encoder, encoder vector, and decoder
- Encoder has LSTM units stacked, each accepting an element from the question
- Encoder vector captures information across the question
- Decoder has a stack of LSTMs each predicting an output
- This model supports varying length input/output though we are starting with a fixed length and using padding



**Figure 10. Seq-to-seq Deep Autoencoder for Learning Translations Between Text and Programs, and Programs and Vectors.**

# Task 4.3 - AI Simulation – Neuro-Symbolic Learning

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- Also, beginning to experiment with the workflow shown in Figure 11
- Starting with experiments that focus on question to program translation
- A model that learns a fixed sized embedding of the question
  - Translatable to programs and readable text
- Based on Neuro-Symbolic Concept Learner

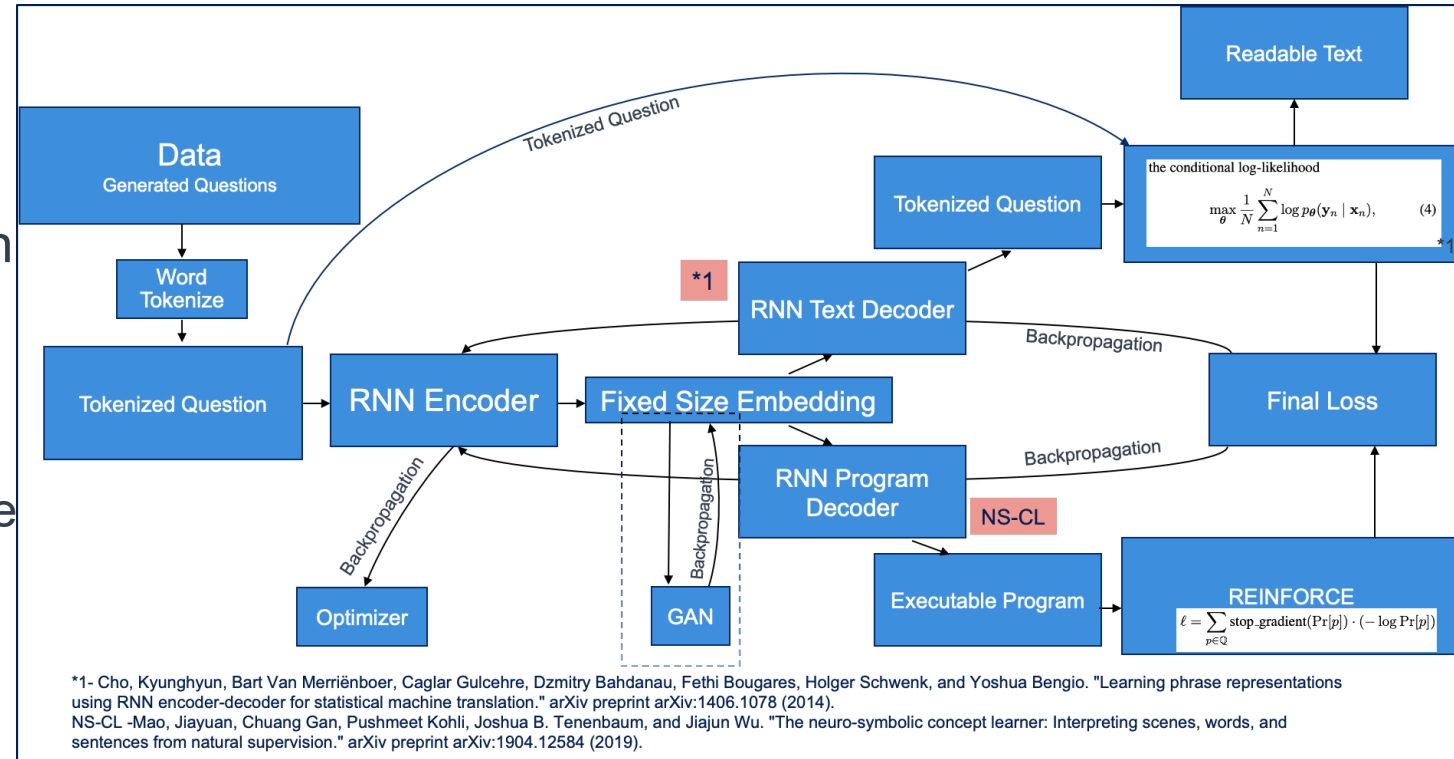
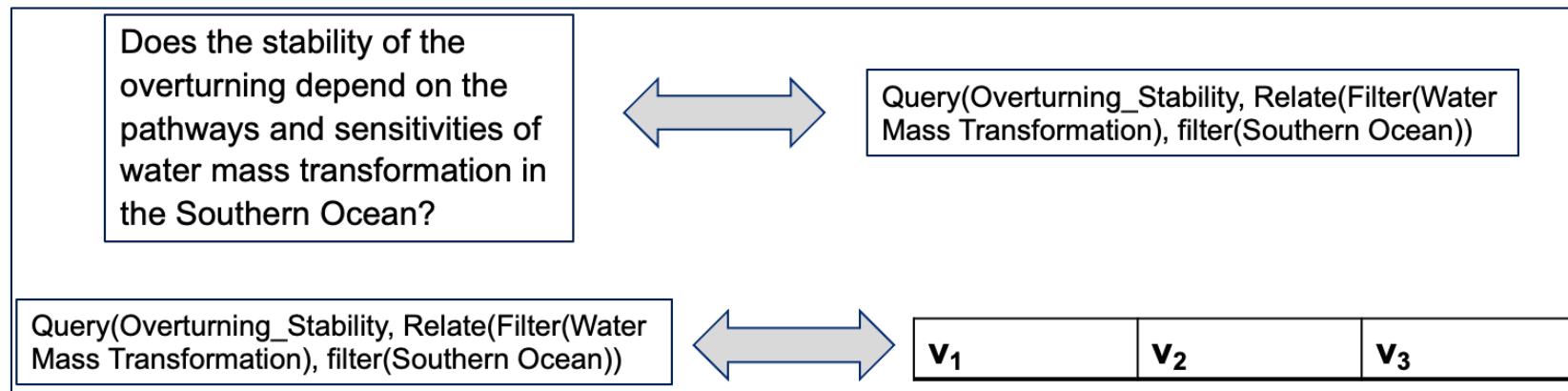


Figure 11. Novel Neuro-Symbolic Architecture for Translating Questions to Programs based on Neuro-Symbolic Concept Learner (NS-CL).

# Task 4.3 - AI Simulation – Neuro-Symbolic Learning

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- Next Steps:
  - Measure performance of the following translations:
    - Questions to programs \*\*
    - Vectors to programs



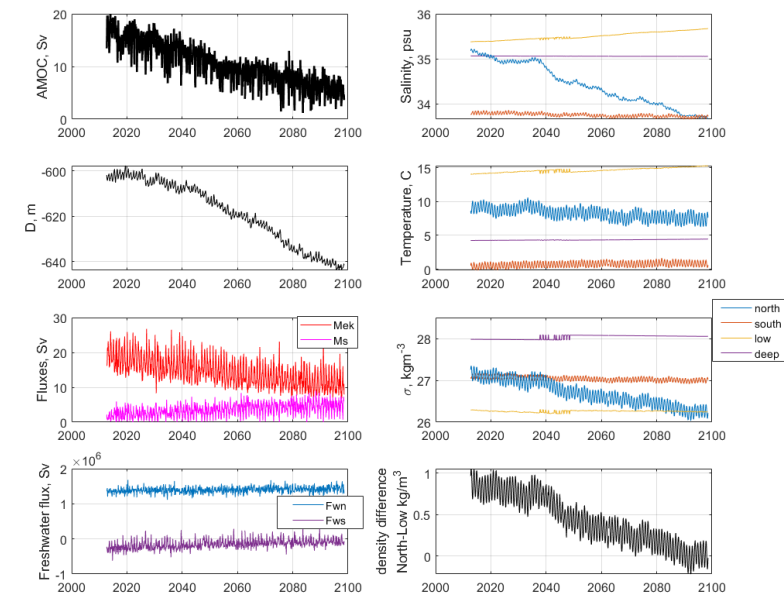
**Figure 12. Visualizing Translations Between Levels – Questions to/from Symbolic Programs (top) and Symbolic Programs to/from Vectors (bottom).**

# Task 4.3 - AI Simulation – Causality – New Insights

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

To address two outstanding issues:

- 1.) AMOC slowing as shown in Figure 13 and inferring likelihood of shutoff, and
  - 2.) Learning how to recover from an AMOC shutoff
- Developing causal inference based on temporal evolution of system state
  - Working on a model to learn relevant causal structures that are occurring as a result of dynamics included in surrogate model
  - Causal model will capture intermediate states along the way to AMOC shutoffs, focusing on particular states that lie at causal forks in the road of the system's temporal evolution and that are most relevant to whether there will be a shutoff or not
  - Will be used to assign probabilities to potential outcomes

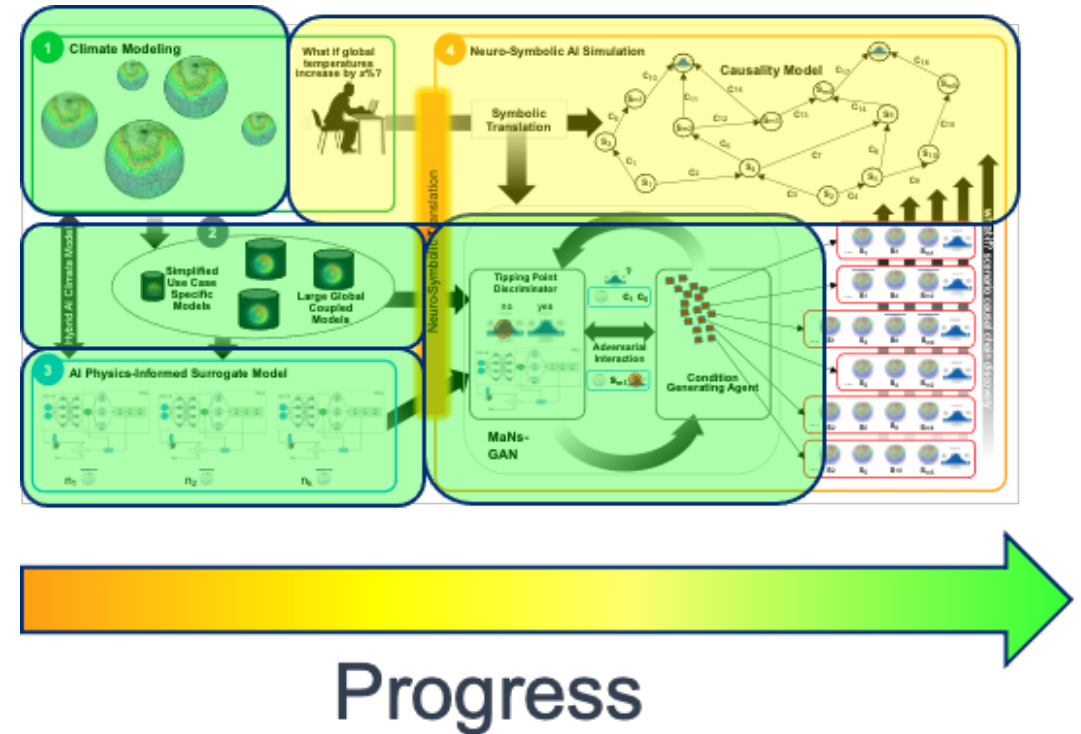


**Figure 13. CESM-2 Model Runs that show weakening of the AMOC.**

# Summary

In summary, we have shared results from our initial experimentation related to the surrogate modeling and the AI simulation, specifically related to the GAN and the neuro-symbolic language.

With Milestone 5, we will continue to push forward with building large GCM calibrated data sets and extensions to the box model.





# JOHNS HOPKINS

APPLIED PHYSICS LABORATORY



# Appendix A

Task 3.3	
<b>Objective</b> AI Physics-Informed Surrogate Learning Formalizations	<b>Task Description</b> Report on the first set of experimental results based on testing the formalizations set forth in Milestone 3.
<b>Primary Organization Responsible</b>	JHU
<b>Human Subjects or Animal Research?</b>	No
<b>Associated Milestones</b>	<b>Deliverables</b>
Milestone 4	Report on 'beta version' of hybrid model analysis including new mathematical insights, along with insights in data analysis.

# Appendix B

Task 4.3	
<b>Objective</b> <b>AI Simulation Formalizations</b>	<b>Subtask Description</b> Report on early experimentation of a baseline GAN for a subset of explorations and what-if questions, including a set of experiments that show feasibility of the causal model, and baseline symbolic language experimental results.
<b>Primary Organization Responsible</b>	<b>APL</b>
<b>Human Subjects or Animal Research?</b>	<b>No</b>
<b>Associated Milestones</b>	<b>Deliverables</b>
<b>Milestone 4</b>	<b>Milestone report – report on 'beta version' of hybrid model analysis including new mathematical insights, along with insights in data analysis.</b>

# Citations

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